Conditioning and Preconditioning in the Cone of SPD matrices

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Joint work with Marcos Raydan (USB, Caracas)

Obervations

- The set $PD_n \subset S_n$ of the $n \times n$ SPD matrices possesses a cone structure
- The Identity matrix Id plays a centrale role : Id is a central ray (Taragaza (90'))
- Angle between matrices reveals as a central tool

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- Angle between matrices reveals as a central tool

Questions

- How to characterize the conditioning of the matrices in PD_n
- How to build (inverse) preconditioners in PD_n

It is natural to use the cosine to measure the angle between two matrices

$$\cos(A, B) = \frac{< A, B >_F}{\|A\|_F \|B\|_F}$$

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The Frobenius condition number of A, $\kappa(A)_F = \|A\|_F \|A^{-1}\|_F$ is then related to the cosine of the angle that A and A^{-1} make with the central ray matrix Id, and also to the angle between A and A^{-1}.

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Of course we would like to avoid to handle quantities with A^{-1} and then produce estimates of the condition number using A only

Properties

Identities and Properties

- $\kappa_F(A)$ expressed with distance between A and A^{-1}

$$\begin{aligned}\kappa(A)_F &= n + \frac{1}{2}\left(\|A - A^{-1}\|_F^2 - (\|A\|_F - \|A^{-1}\|_F)^2\right)\\ &= n + \frac{1}{2}D(A, A^{-1}).\end{aligned}$$

- $$1 + \frac{1}{2n}D(A, A^{-1}) \leq \kappa_2(A) \leq n + \frac{1}{2}D(A, A^{-1})$$

- $$\frac{1}{\kappa_2(A)} \leq \cos(A, A^{-1}) \leq \cos(A, Id)\cos(A^{-1}, Id)$$

Properties (segue)

Properties

- $$\frac{1}{n} \leq \frac{\cos(A, Id)}{\cos(A^{-1}, Id)} \leq n$$
- $$\kappa_F(A) \geq \max(n, \frac{\sqrt{n}}{\cos^2(A, Id)})$$
- (Wolfowicz & Styan, 80') with $m = tr(A)/n, p = \sqrt{n-1}, s^2 = \|A\|_F^2/n - m^2$,
$$\kappa_F(A) \geq \mathrm{Max}\left(n, \frac{\sqrt{n}}{\cos^2(A, Id)}, \left(1 + \frac{2s}{m - \frac{s}{p}}\right)\right)$$

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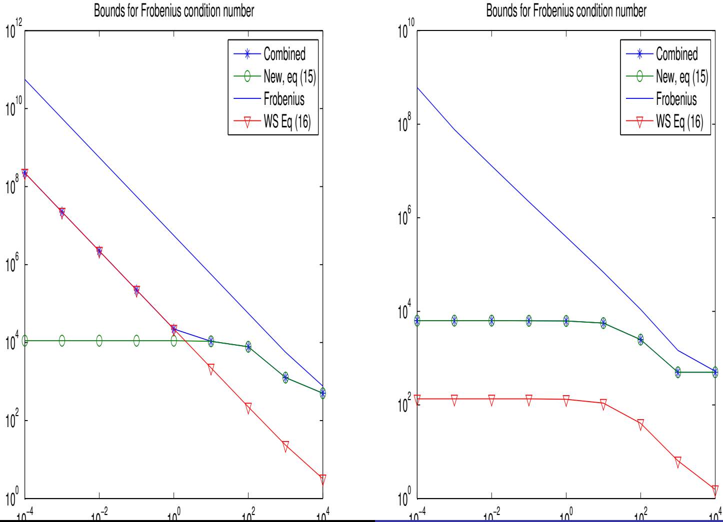
Rmk : Statistical interpretation with $M = m\ Id$, spectral mean value matrix of A and $s^2 = \|A - M\|_F^2/n$ is the variance, $\frac{s}{p}$ is the unbiased standard deviation.

Illustration



Approximation of the inverse using the Cosine

Let X_k be a sequence of matrices, then

$$\|Id - X_k A\|_F^2 = (\|Id\|_F - \|X_k A\|_F)^2 + 2(1 - \cos(Id, X_k A))\|Id\|_F \|X_k A\|_F$$

Then is X_k, is a sequence of matrices converging to A^{-1} assuming that $\|X_k A\|_F = \sqrt{n} = \|Id\|_F$, we have

$$\|Id - X_k A\|_F^2 = 2n(1 - \cos(Id, X_k A))$$

IDEA : build X_k as minimizing sequence of $F(X) = 1 - \cos(Id, XA)$
Rmk : we could consider also $F_1(X) = 1 - \cos(Id, AX)$.

As seen above, these sets will play an important role

$$S = \{X \in \mathcal{M}_n(\mathbb{R}) / \|XA\|_F = \sqrt{n}\}, \; T = \{X \in \mathcal{M}_n(\mathbb{R}) / tr(XA) \geq 0\}$$

- $F(X) = 0 \Longrightarrow X = \xi A^{-1}, \xi > 0$
- $F(X) = 0$ and $X \in S \Longrightarrow X = A^{-1}$

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Important remark : $F(X)$ is invariant by positive scaling, say

$$F(\alpha X) = F(X)$$

This will give the boundness of approximating sequences of matrices when working in S

Basic properties of F and S

- $\nabla F(X) = \dfrac{1}{\|Id\|_F \|XA\|_F} \left(\dfrac{< XA, Id >}{\|XA\|_F^2} XA - Id \right) A^T$
- $< \nabla F(X), X >= 0, \forall X \in S$
- $\dfrac{\sqrt{n}}{\|A\|_F} \leq \|X\|_F \leq \sqrt{n} \|A^{-1}\|_F, X \in S$

Negative gradient direction

- Iterations

$$X^{(k+1)} = X^{(k)} - \alpha_k \nabla F(X^{(k)}),$$

- Steepest descent : optimal α_k that optimizes $F(X^{(k)} + \alpha D_k)$, is

$$\alpha_k = \frac{\left(\langle X^{(k)}A, I\rangle \langle X^{(k)}A, D_k A\rangle - n\,\langle D_k A, I\rangle\right)}{\left(\langle D_k A, I\rangle \langle X^{(k)}A, D_k A\rangle - \langle X^{(k)}A, I\rangle \langle D_k A, D_k A\rangle\right)}.$$

- Since $\|I\|_F = \sqrt{n}$,

$$X^{(k+1)} = X^{(k)} - \frac{\alpha_k}{\sqrt{n}\,\|X^{(k)}A\|_F}\left(\frac{\langle X^{(k)}A, I\rangle}{\|X^{(k)}A\|_F^2} X^{(k)}A - I\right)A,$$

imposing the condition $\|X^{(k)}A\|_F = \sqrt{n}$,

$$X^{(k+1)} = X^{(k)} - \frac{\alpha_k}{n}\left(\frac{\langle X^{(k)}A, I\rangle}{n} X^{(k)}A - I\right)A,$$

Algorithm 1 : CauchyCos (Steepest descent approach on $F(X) = 1 - \cos(XA, I)$)

Given $X_0 \in PSD$
for $k = 0, 1, \cdots$ until a stopping criterion is satisfied, **do**
  Set $w_k = \langle X^{(k)}A, I\rangle$
  Set $\nabla F(X^{(k)}) = \frac{1}{n}\left(\frac{w_k}{n}X^{(k)}A - I\right)A$
  Set $\alpha_k = \left|\frac{n\,\langle \nabla F(X^{(k)})A, I\rangle - w_k\langle X^{(k)}A, \nabla F(X^{(k)})A\rangle}{\langle \nabla F(X^{(k)})A, I\rangle\langle X^{(k)}A, \nabla F(X^{(k)})A\rangle - w_k\|\nabla F(X^{(k)})A\|_F^2}\right|$
  Set $Z^{(k+1)} = X^{(k)} - \alpha_k \nabla F(X^{(k)})$
  Set $X^{(k+1)} = s\sqrt{n}\frac{Z^{(k+1)}}{\|Z^{(k+1)}A\|_F}$, where $s = 1$ if $trace(Z^{(k+1)}A) > 0$, $s = -1$ else
end for

Lemma

If $X^{(0)}A = AX^{(0)}$, then $X^{(k)}A = AX^{(k)}$, for all $k \geq 0$ in the CauchyCos Algorithm.

Lemma

If $X^{(0)}A = AX^{(0)}$, then the sequences $\{X^{(k)}\}$, $\{Z^{(k)}\}$, and $\{Z^{(k)}A\}$ generated by the CauchyCos Algorithm are uniformly bounded away from zero.

Theorem

The sequence $\{X^{(k)}\}$ generated by the CauchyCos Algorithm converges to A^{-1}.

To avoid oscillation of the steepest descent : right preconditioning

$$\widehat{D}_k \equiv \widehat{D}(X^{(k)}) = -\frac{1}{n}\left(\frac{\langle X^{(k)}A, I\rangle}{n} X^{(k)}A - I\right), \qquad (1)$$

Rmk : MINRES can be seen as a steepest descent inverse-right-preconditioned by $(A^T)^{-1}$.

Algorithm 2 : MinCos (simplified gradient approach on $F(X) = 1 - \cos(XA, I)$)

Given $X_0 \in PSD$

for $k = 0, 1, \cdots$ until a stopping criterion is satisfied, **do**

  Set $w_k = \langle X^{(k)}A, I\rangle$

  Set $\widehat{D}_k = -\frac{1}{n}\left(\frac{w_k}{n}X^{(k)}A - I\right)$

  Set $\alpha_k = \left|\frac{n\,\langle \widehat{D}_k A, I\rangle - w_k \langle X^{(k)}A, \widehat{D}_k A\rangle}{\langle \widehat{D}_k A, I\rangle\langle X^{(k)}A, \widehat{D}_k A\rangle - w_k \|\widehat{D}_k A\|_F^2}\right|$

  Set $Z^{(k+1)} = X^{(k)} + \alpha_k \widehat{D}_k$

  Set $X^{(k+1)} = s\sqrt{n}\frac{Z^{(k+1)}}{\|Z^{(k+1)}A\|_F}$, where $s = 1$ if $trace(Z^{(k+1)}A) > 0$, $s = -1$ else

end for

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To produce iterates that belong in $\mathcal{S}$, we apply a sparsification (e.g. by thresholding the coefficients) to $Z^{(k+1)}$, before the rescaling, say

Algorithm 4 : Sparsified iterates

1: **Set** $Z^{(k+1)} = X^{(k)} + \alpha_k \widehat{D}_k$
2: **Sparsify** $Z^{(k+1)}$ as $\mathcal{Z}^{(k+1)} = \mathcal{F}(Z^{(k+1)})$
3: **Set** $X^{(k+1)} = s\sqrt{n}\dfrac{\mathcal{Z}^{(k+1)}}{\|\mathcal{Z}^{(k+1)}A\|_F}$

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3: **Set** $X^{(k+1)} = s\sqrt{n}\dfrac{\mathcal{Z}^{(k+1)}}{\|\mathcal{Z}^{(k+1)}A\|_F}$

The sparsification wil be realized by using a threshold tolerance, combined with a fixed bound on the maximum number of nonzero elements to be kept at each column (or row) to limit the fill-in.

Algorithm 6 : Sparse MinCos

Given $X_0 \in PSD$
for $k = 0, 1, \cdots$ until a stopping criterion is satisfied, **do**
  Set $w_k = \langle X^{(k)}A, I \rangle$
  Set $\widehat{D}_k = -\frac{1}{n}\left(\frac{w_k}{n}X^{(k)}A - I\right)$
  Set $\alpha_k = \left| \dfrac{n\,\langle \widehat{D}_k A, I\rangle - w_k \langle X^{(k)}A, \widehat{D}_k A\rangle}{\langle \widehat{D}_k A, I\rangle \langle X^{(k)}A, \widehat{D}_k A\rangle - w_k \|\widehat{D}_k A\|_F^2} \right|$
  Set $Z^{(k+1)} = X^{(k)} + \alpha_k \widehat{D}_k$
  Sparsify $Z^{(k+1)}$ as $\mathcal{Z}^{(k+1)} = \mathcal{F}(Z^{(k+1)})$
  Set $X^{(k+1)} = s\sqrt{n}\dfrac{\mathcal{Z}^{(k+1)}}{\|\mathcal{Z}^{(k+1)}A\|_F}$, where $s = 1$ if $trace(\mathcal{Z}^{(k+1)}A) > 0$, $s = -1$ else
end for

Numerical Results

The examples

- from the Matlab gallery : Poisson, Lehmer, Wathen, Moler, and minij. Notice that the Poisson matrix, referred in Matlab as (Poisson, N) is the $N^2 \times N^2$ finite differences 2D discretization matrix of the negative Laplacian on $]0,1[^2$ with homogeneous Dirichlet boundary conditions.
- Poisson 3D (that depends on the parameter N), is the $N^3 \times N^3$ finite differences 3D discretization matrix of the negative Laplacian on the unit cube with homogeneous Dirichlet boundary conditions.
- from the Matrix Market : nos1, nos2, nos5, and nos6.

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The methods

- minimizing $F(X)$: CauchyCos (Steepest), MinCos (right Prec. Steepest)
- minimizing $\Phi(X) = \frac{1}{2}\|I - XA\|_F^2$: CauchyFro (Steepest), MinRes (right. Prec Steepest)
- Stopping criteria $Min(\Phi(X^{(k)}), F(X^{(k)})) \leq \epsilon$

Matrix A	Size $(n \times n)$	$\kappa(A)$	A
Poisson (50)	n=2500	1.05e+03	sparse
Poisson (100)	n=1000	6.01e+03	sparse
Poisson (150)	n=22500	1.34e+04	sparse
Poisson (200)	n=40000	2.38e+04	sparse
Poisson 3D (10)	n=1000	79.13	sparse
Poisson 3D (15)	n=3375	171.66	sparse
Poisson 3D (30)	n=27000	388.81	sparse
Poisson 3D (50)	n=125000	1.05e+03	sparse
Lehmer (100)	n=100	1.03e+04	dense
Lehmer (200)	n=200	4.2e+04	dense
Lehmer (300)	n=300	9.5e+04	dense
minij (100)	n=100	1.63e+04	dense
minij (200)	n=200	6.51e+04	dense
moler (100)	n=100	3.84e+16	dense
moler (200)	n=200	3.55e+16	dense
nos1	n=237	2.53e+07	sparse
nos2	n=957	6.34e+09	sparse
nos5	n=468	2.91e+04	sparse
nos6	n=675	8.0e+07	sparse

Matrix	Size ($n \times n$)	CauchyCos	CauchyFro	MinRes	MinCos
Poisson 2D (50)	n=2500	88	132	7	6
Poisson 3D (10)	n=1000	9	12	3	2
Poisson 3D (15)	n=3375	10	14	3	2
Lehmer (10)	n=10	888	1141	21	15
Lehmer (20)	n=20	9987	49901	123	51
Minij (20)	n=20	31271	63459	209	45
Minij (30)	n=30	153456	629787	553	102
Moler (100)	n=100	7	83	3	3
Moler (200)	n=200	77	15243	19	12
Wathen (10)	n=341	10751	17729	68	57
Wathen (20)	n=1281	495	1112	22	16

Table : Number of iterations required for all considered methods when $\epsilon = 0.01$.

Matrix	Size ($n \times n$)	CauchyCos	CauchyFro	MinRes	MinCos
Poisson 2D (100)	n=1000			7	7
Poisson 2D (200)	n=40000			7	7
Poisson 3D (30)	n=27000			3	3
Poisson 3D (50)	n=125000			3	3
Lehmer (50)	n=50			987	293
Lehmer (70)	n=70			1399	423
Lehmer (100)	n=100			3905	1178
Lehmer (200)	n=200			16189	4684
Minij (100)	n=100			6771	1259
Minij (200)	n=200			26961	5057
Moler (300)	n=300			105	22
Moler (500)	n=500			381	48
Moler (1000)	n=1000			1297	152
Wathen (30)	n=2821			24	17
Wathen (50)	n=7701			20	15

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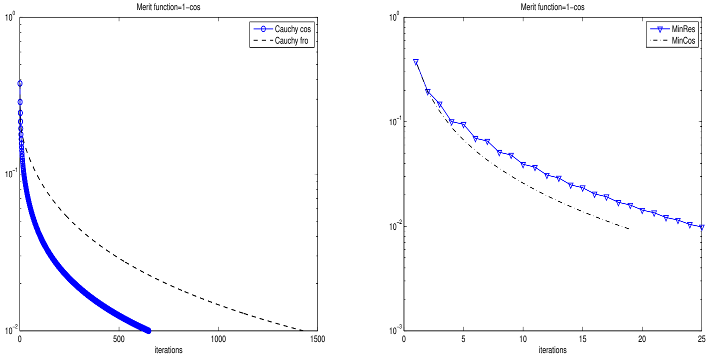

Figure : Convergence history for CauchyFro and CauchyCos (left), and MinRes and MinCos (right) for $F(X)$ (up), when applied to the Wathen matrix for $n = 20$ and $\epsilon = 0.01$.

Sparse approximation

The sparsification is based on a threshold tolerance with a limited fill-in (*lfil*) on the matrix $Z^{(k+1)}$, at each iteration, before the scaling step to guarantee that the iterate $X^{(k+1)} \in S \cap T$.

- *thr* as the percentage of coefficients less than the maximum value of the modulus of all the coefficients in a column
- for each i-th column we select at most *lfil* off-diagonal coefficients among the ones that are larger in magnitude than $thr \times \|(Z^{(k+1)})_i\|_\infty$, where $(Z^{(k+1)})_i$ represents the i-th column of $Z^{(k+1)}$.

Matrix	Method	$\kappa(X^{(k)}A)/\kappa(A)$	$[\lambda_{min}, \lambda_{max}]$ of $(X^{(k)}A)$	Iter	% fill-in
nos1 ($lfil = 10$)	MinCos	0.0835	[2.44e-06,2.3272]	20	3.71
nos1($lfil = 10$)	MinRes		[-98.66,5.40]		
nos6 ($lfil = 10$)	MinCos	0.4218	[5.07e-06,3.1039]	20	0.45
nos6 ($lfil = 20$)	MinCos	0.2003	[8.51e-06,3.0702]	20	0.82
nos6($lfil = 10$)	MinRes		[-0.7351,2.6001]		
nos6($lfil = 20$)	MinRes		[-0.2256,2.2467]		
nos5($lfil = 5$)	MinCos	0.068	[0.002,1.36]	10	1.18
nos5($lfil = 10$)	MinCos	0.0755	[00.0024,1.3103]	10	2.47
nos5($lfil = 5$)	MinRes		[-20.31,2.16]		
nos5($lfil = 10$)	MinRes	0.1669	[0.0021,1.7868]	10	2.36
nos2($lfil = 5$)	MinCos	0.1289	[5.2e-09,2.73]	10	0.52
nos2($lfil = 10$)	MinCos	0.0891	[7.95e-09,2.2873]	10	0.80
nos2($lfil = 20$)	MinCos	0.0700	[9.7e-09,1.9718]	10	1.14
nos2($lfil = 5$)	MinRes		$[-0.3326, 2.4869]$		
nos2($lfil = 10$)	MinRes	0.0970	[4.21e-09,1.5414]	10	0.93
nos2($lfil = 20$)	MinRes	0.0861	[4.21e-09,1.1638]	10	1.14

Table : Performance of MinRes and MinCos when applied to the Matrix Market matrices nos1, nos2, nos5, and nos6, for $\epsilon = 0.01$, $thr = 0.01$, and different values of $lfil$.

Matrix A	Size $(n \times n)$	$\kappa(X^{(k)}A)/\kappa(A)$	$[\lambda_{min}, \lambda_{max}]$ of $(X^{(k)}A)$	iter	% fil-in
wathen (30)	n=2821	0.0447	$[0.0109, 1.3889]$	20	0.73
wathen (50)	n=7701	0.0461	$[0.0366, 1.4012]$	20	0.27
wathen (70)	n=14981	0.0457	$[0.0086, 1.3894]$	20	0.14
wathen (100)	n=30401	0.0467	$[0.0289, 1.4121]$	20	6.8436e-02

Table : Performance of MinCos applied to the Wathen matrix for different values of n and a maximum of 20 iterations, when $\epsilon = 0.01$, $thr = 0.04$, and $lfil = 20$.

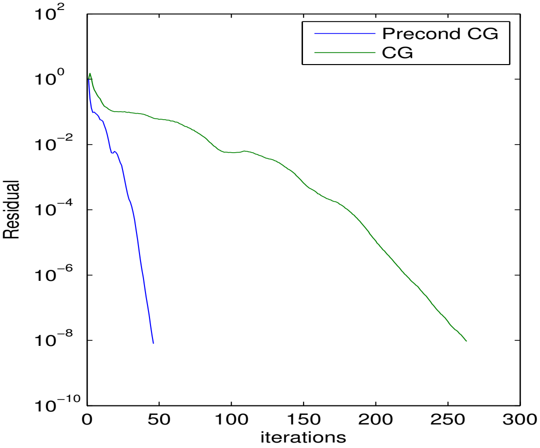

Figure : Convergence history of the CG method applied to a linear system with the Wathen matrix, for $n = 50$, 20 iterations, $\epsilon = 0.01$, $thr = 0.01$, and $lfil = 20$, using the preconditioned generated by the MinCos Algorithm and without preconditioning.

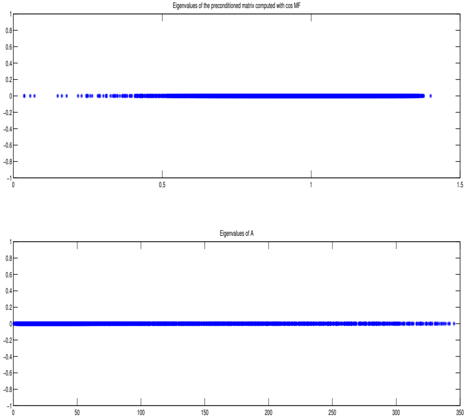

Figure : Eigenvalues distribution of A (down) and of $X^{(k)}A$ (up) after 20 iterations of the MinCos Algorithm when applied to the Wathen matrix for $n = 50$, $\epsilon = 0.01$, $thr = 0.01$, and $lfil = 20$.

- The angle between a Matrix A and the identity in $C \cap S$ is a way to study the condition number of A
- The approximations to the inverse are built in a nonlinear set and take advantage of induced properties
- The gradient method is nothing else but a Forward Euler's scheme applied to a gradient flow

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  - Gradient flows and Backward Euler's method to compute minimizers of a functional using **L**ojasewicz inequality (M. Pierre & B. Merlet for linear spaces (2010), B. Merlet & T.N. Nguyen for manifolds, 2013)
  - Literature : gradient methods on manifolds (Projected Gardient methods along geodesiscs, A. Lichnewsky (1979)), Optimization Algorithms on Matrix Manifolds (Mahony *et al*, AMS 2007)